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14. ABSTRACT
Heterogeneous catalysis is studied both theoretically and experimentally employing neutral gas phase metal and metal compound clusters as the active catalytic species. The techniques involve laser ablation of metals and metal compounds to form neutral clusters, supersonic expansion to cool them, reaction in a fast flow reactor with small molecules, single photon ionization for time of flight mass spectrometry to detect reactants, intermediates, and products, and theory to calculate a mechanistic reaction potential energy surface. Many reactions have been studied in this manner and their mechanisms have been generated, lending to a presentation of a full condensed phase catalytic cycle. Some representative reactions are SO2 to SO3, CO and H2 to methanol, CO to CO2, NO and NH3 to N2 and H2O, O2 and C2 H2 and C4H4 to generate CH2CO and CH3CHO, methanol oxidation to H2CO, C=C bond cleavage, and generation of the new cluster systems AlmCnHx, MgmCnHx, and BemCnHx for potential energy applications.

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The basic idea behind this research is that condensed phase heterogeneous catalytic reactions are driven by localized structures on surfaces and in the bulk. These moieties can be generated by clusters synthesized, isolated, and cooled in the gas phase: they can react with the same molecules for which the condensed phase catalysts are active. These reactions are then studied by mass spectrometry and theoretical techniques to generate: reactive species; reaction mechanisms; reaction potential energy surfaces; and complete catalytic cycles for the condensed phase reactions and behaviors. Once such fundamental information is known for a catalytic process, new catalysts can be designed and old ones can be greatly improved as the active species can be enhanced and/or emphasized for the given process of interest. Our program is unique in the respect that our study is for neutral systems, which we have learned to access, without fragmentation, by mass spectrometry. We have demonstrated this in many publications through 6.4, 10.5, 26.5 eV single photon ionization of reactants and products.

The clear and achieved goals of this program are the following: 1. determine the active cluster species for the given catalytic reactions; 2. determine the reaction mechanism for the generation of desired products; 3. generate a complete catalytic cycle for the reaction of interest; 4. propose improved and new catalytic systems to generate desired products from simple reactants and readily available catalyst materials.

In the program we have found three different general types of catalytic species for characterization: 1. oxidation/reduction catalysts for which some catalytic sites are reduced (oxygen rich sites) and some catalytic sites are oxidized

(oxygen deficient sites) and together they generate a complete catalytic cycle (e.g., $V_mO_m + SO_2 \rightarrow SO/SO_3 + V_mO_n$); 2. specific active sites that are catalytic (e.g., $Nb_8 + CO + H_2 \rightarrow Nb_8 + CH_3OH$); and 3. facilitation catalysts such that the catalyst generally accommodates two species that are brought together on its sites and react (e.g., ($V_mO_m + NO + NH_3 + O_2 \rightarrow V_mO_m + N_2 + H_2O$).

Below we present some of the detailed reaction systems we have studied and published on over the last grant period.

1. Reactions OF NEUTRAL VANADIUM AND TANTALUM OXIDE CLUSTERS with NO and NH_3

Reactions of neutral vanadium and tantalum oxide clusters with NO_x, NH_3, and an NO/NH_3 mixture in a fast flow reactor are investigated by time of flight mass spectrometry and density functional theory (DFT) calculations. Single photon ionization through a 46.9 nm (26.5 eV) soft x-ray (SXR) laser is employed to detect both neutral cluster distributions and reaction products. Very few association products are detected for V_mO_n clusters reacting with pure NO. Only the products VO_3NO and V_2O_5NO are observed. No reactions (adsorptions) with NO_2 are detected for V_mO_n clusters. On the other hand, the Ta_mO_n cluster system is found to generate many reaction products, $TaO_{3,4}(NO)_{1,2}$, Ta_2O_5NO, $Ta_2O_6(NO)_{1\text{-}3}$, and $Ta_3O_8(NO)_{1,2}$. A similar adsorption reaction occurs for NO_2 with Ta_mO_n clusters. Both V_mO_n and Ta_mO_n cluster systems are very active with NH_3. The main products of the reaction with NH_3 result from the adsorption of one or two NH_3 molecules on the respective clusters. A few products are observed with extra hydrogen(s) (e.g., $Ta_2O_5(NH_3)H$). A gas mixture of NO:NH3 (9:1) is also added to the fast flow reactor: the V_mO_n cluster system apparently behaves as if only NH_3 were present in the reactor, as no combined NH_3/NO adducts or reactions are detected; and Ta_mO_n clusters form adducts with the gas mixture generating products such as $TaO_{2,3}NH_3NO$, and $Ta_2O_5(NH_3)_{1,2}NO$. The mechanisms for the reactions of neutral V_mO_n and Ta_mO_n clusters with NO/NH_3 are explored via DFT calculations. The calculations give an interpretation of the data that is consistent with the condensed phase reactivity of a V_mO_n catalyst and suggest formation of intermediates in the catalytic chemistry. Based on this gas phase chemistry, a catalytic cycle is proposed for the overall reaction: $N_2 + NH_3 + O_2 \rightarrow N_2 + H_2$.

2.Oxidation reactions on neutral cobalt oxide clusters on neutral V_mO_m.

Reactions of neutral cobalt oxide clusters (Co_mO_n, m = 3-9, n = 3-13) with CO, NO, SO_2, C_2H_2, and C_2H_4 to produce CO_2, NO_2, SO_3, CH_2CO, and CH_3CHO in a fast flow reactor are investigated by time of flight mass spectrometry employing 118 nm (10.5 eV) single photonionization. Strong cluster size dependent behavior is observed for all the oxidation reactions; the Co_3O_4 cluster has the highest reactivity

for reactions with CO, NO, and SO_2. Cluster reactivity is also highly correlated with cluster size, Co(III) concentration, the number of the cobalt atoms with high oxidation states, and the presence of an oxygen molecular moiety in the Co_mO_n clusters. The experimental cluster observations are in good agreement with condensed phase Co_3O_4 behavior. Density functional theory calculations at the BPW91/TZVP level are carried out to explore the geometric and electronic structures of the Co_3O_4 cluster, reaction intermediates, transition states, as well as reaction mechanisms. CO, NO, SO_2, C_2H_2, and C_2H_4 are predicted to be adsorbed on the Co(II) site, and react with one of the parallel bridge oxygen atoms between two Co(III) atoms in the Co_3O_4 cluster. All studied oxidation reactions on the Co_3O_4 cluster are estimated as thermodynamically favorable and overall barrierless processes at room temperature. The oxygen centered radicals in the Co_3O_4 cluster are responsible for the oxidation reactions with CO, NO, SO_2, C_2H_2, and C_2H_4. Based on the gas phase experimental and theoretical cluster studies, a catalytic cycle for these oxidation reactions on a condensed phase cobalt oxide catalyst is proposed.

3. Reactions of Neutral Vanadium Oxide Clusters with Methanol

Single-photon ionization through soft X-ray (46.9 nm, 26.5 eV) and vacuum ultraviolet (VUV, 118 nm, 10.5 eV) lasers is employed to detect both neutral cluster distributions and reaction products. In order to distinguish isomeric products generated in the reactions V_mO_n + CH_3OH, partially deuterated methanol (CD3OH) is also used as a reactant in the experiments. Association products are observed for most vanadium oxide clusters in reaction with methanol. Products VOD, V_2O_3D, V_3O_6D, and V_4O_9D are observed for oxygen-deficient vanadium oxide clusters reacting with methanol, while oxygen rich and the most stable clusters can extract more than one hydrogen atom (H/D) from CD_3OH to form products $VO_2DH_{0,1}$, $V_2O_4DH_{0,1}$, $V_2O_5DH_{0,1}$, $V_3O_7DH_{0,1}$, and $V_4O_{10}DH_{0,1}$. Species $VO_2(CH_3)2$, $VO_3(CH_3)_2$, $V_2O_5(CH_3)_2$, $V_3O_7(CH_3)_2$, and $V_3O_8(CH_3)_2$ are identified as some of the main products generated from a dehydration reaction for V_mO_n + CH_3OH. A minor reaction channel that generates $VOCH_2O$ ($VOCD_2O$) and VO_2CH_2O (VO_2CD_2O) can also be identified. An obviously different behavior appears in the reaction V_mO_n + C_2H_5OH. The main observed products for this reaction are association products of the form $V_mO_nC_2H_5OH$. In order to explore the mechanism of V_mO_n + CH_3OH reactions, DFT calculations are performed to study the reaction pathways of VO_2 + CH_3OH and VO + CH_3OH reaction systems. The calculation results are in good agreement with the experimental observations.

4. Reactions of small neutral iron oxide clusters with methanol

Detection of the neutral iron oxide cluster distribution and reaction intermediates and products is accomplished through single photonionization by a 118 nm, 10.5 eV VUV laser. Partially deuterated methanol CD3OH is employed to distinguish reaction products and reaction mechanisms. Three major reactions are identified experimentally: CH_3OH association with FeO; methanol dehydrogenation on $FeO_{1,2}$ and Fe_2O_{2-5}; and CH_2OFe formation. Density functional theory calculations are

carried out to identify reaction products, and to explore the geometric and electronic structures of the iron oxide clusters, reaction intermediates, and transition states, and to evaluate reaction pathways. Neutral formaldehyde is calculated to be formed on $FeO_{1,2}$ and Fe_2O_{2-5} clusters. Hydrogen transfer from methanol to iron oxide clusters occurs first from the O–H moiety of methanol, and is followed by a hydrogen transfer from the C–H moiety of methanol. Computational results are in good agreement with experimental observations and reveal reaction mechanisms for neutral iron oxide clusters taking methanol to formaldehyde through various reaction intermediates. Based on the experimental results and the calculated reaction mechanisms and pathways, complete catalytic cycles are suggested for the heterogeneous reaction of CH_3OH to CH_2O facilitated by an iron oxide catalyst.

5. C=C Bond Cleavage on Neutral $VO_3(V_2O_5)_n$ Clusters

The reactions of neutral vanadium oxide clusters with alkenes (ethylene, propylene, 1-butene, and 1,3-butadiene) are investigated. Single photon ionization through extreme ultraviolet radiation (EUV, 46.9 nm, 26.5 eV) is used to detect neutral cluster distributions and reaction products. Products $(V_2O_5)_nVO_2CH_2$, $(V_2O_5)_nVO_2C_2H_4$, $(V_2O_5)_nVO_2C_3H_4$, and $(V_2O_5)nVO_2C_3H_6$, for neural V_mO_n clusters in reactions with C_2H_4, C_3H_6, C_4H_6, and C_4H_8, respectively are observed. The observation of these products indicates that the C=C bonds of alkenes can be broken on neutral oxygen rich vanadium oxide clusters with the general structure $VO_3(V_2O_5)$ n = 0,1,2.... DFT calculations demonstrate that the reaction $VO_3 + C_3H_6 \rightarrow VO_2C_2H_4 + H_2CO$ is thermodynamically favorable and overall barrierless at room temperature. They also provide a mechanistic explanation for the general reaction in which the C=C double bond of alkenes is broken on $VO_3(V_2O_5)_n$ n=0,1,2...clusters. A catalytic cycle for alkene oxidation on vanadium oxide is suggested based on our experimental and theoretical investigations. The reactions of V_mO_n with C_6H_6 and C_2F_4 are also investigated by experiments. The products $2(V_2O_5)_nC_6H_4$ are observed for dehydration reactions between V_mO_n clusters and C_6H_6. No product is detected for V_mO_n clusters reacting with C_2F_4. The mechanisms of the reactions between VO_3 and C_2F_4/C_6H_6 are also investigated by calculations at the B3LYP/TZVP level.

6. Reactions of Sulfur Dioxide with Neutral Vanadium Oxide Clusters in the Gas Phase.

Single-photon ionization through vacuum ultraviolet (VUV, 10.5 eV) and soft X-ray (extreme ultraviolet, EUV, 26.5 eV) laser radiation is successfully employed for the study of the reactions of neutral vanadium oxide clusters V_mO_n with sulfur dioxide (SO_2) in the gas phase. V_mO_n clusters are generated by reaction of a laser generated vanadium plasma with O_2 in a supersonic expansion. The clusters are cooled in the expansion and are reacted with SO_2 in a fast-flow reactor. Detection of neutral clusters and products is through ionization employing VUV and EUV laser radiation and time-of-flight mass spectrometry. Many association reaction intermediates [$V_mO_nSO_2$ and $V_2O_4(SO_2)_2$] are observed. Isolated SO is also observed, as a product as

predicted by theoretical studies presented in part I (J. Phys. Chem. A 2007, 111, 13339). A weak feature at the SO3 mass channel (80 amu) is suggested to be present in the product mass spectra. Further reactions of the intermediates with O_2 are positively identified for VO_2SO_2, $V_3O_7SO_2$, and $V_5O_{10}SO_2$. Reaction mechanisms are interpreted on the basis of the observations and preliminary theoretical calculations. Molecular level reaction mechanisms for oxidation of SO_2 to SO_3 facilitated by condensed-phase vanadium oxides as catalysts are suggested.

7. Partial Oxidation of Propylene Catalyzed by VO_3 Clusters

Density functional theory (DFT) calculations are carried out to investigate partial oxidation of propylene over neutral VO3 clusters. C=C bond cleavage products $CH_3CHO + VO_2CH_2$ and $HCHO + VO_2CHCH_3$ can be formed overall barrierlessly from the reaction of propylene with VO_3 at room temperature. Formation of hydrogen transfer products $H_2O + VO_2C_3H_4$, $CH_2{=}CHCHO + VO_2H_2$, $CH_3CH_2CHO + VO_2$, and $(CH_3)_2CO + VO_2$ is subject to tiny (0.01 eV) or small (0.06 eV, 0.19 eV) overall free energy barriers, although their formation is thermodynamically more favorable than the formation of C=C bond cleavage products. These DFT results are in agreement with recent experimental observations. VO_3 regeneration processes at room temperature are also investigated through reaction of O_2 with the C=C bond cleavage products VO_2CH_2 and VO_2CHCH_3. The following barrierless reaction channels are identified: $VO_2CH_2 + O_2 \rightarrow VO_3 + CH_2O$; $VO_2CH_2 + O_2 \rightarrow VO_3C + H_2O$, $VO_3C + O_2 \rightarrow VO_3 + CO_2$; $VO_2CHCH_3 + O_2 \rightarrow VO_3 + CH_3CHO$; and $VO_2CHCH_3 + O_2 \rightarrow VO_3C + CH_3OH$, $VO_3C + O_2 \rightarrow VO_3 + CO_2$. The kinetically most favorable reaction products are CH_3CHO, H_2O, and CO_2 in the gas phase model catalytic cycles. The results parallel similar behavior in the selective oxidation of propylene over condensed phase V_2O_5/SiO_2 catalysts.

8. Density Functional Theory Study of Small Vanadium Oxide Clusters

Density functional theory is employed to study structure and stability of small neutral vanadium oxide clusters in the gas phase. BPW91/LANL2DZ level of theory is used to obtain structures of VO_y (y = 1-5), V_2O_y (y = 2-7), V_3O_y (y = 4-9), and V_4O_y (y = 7-12) clusters. Enthalpies of growth and fragmentation reactions of the lowest energy isomers of vanadium oxide molecules are also obtained to study the stability of neutral vanadium oxide species under oxygen saturated, gas-phase conditions. Our results suggest that cyclic and cage-like structures are preferred for the lowest energy isomers of neutral vanadium oxide clusters, and oxygen-oxygen bonds are present for oxygen-rich clusters. Clusters with an odd number of vanadium atoms tend to have low spin ground states, while clusters with even number of vanadium atoms have a variety of spin multiplicities for their ground electronic state. VO_2, V_2O_5, V_3O_7, and V_4O_{10} are predicted to be the most stable neutral clusters under oxygen saturated conditions. These results are in agreement with and complement previous gas-phase experimental studies of neutral vanadium oxide clusters.

9. Reactivity of optical coating materials with hydrocarbons by use of a desktop-size extreme-ultraviolet laser

The reactivity of prospective capping-layer extreme-ultraviolet (EUV) mirror materials with hydrocarbons is studied in the gas phase by use of mass spectroscopy of metal-oxide clusters. We report the results of chemistry studies for Si_m, Ti_m, Hf_m, and Zr_mO_n metal oxide clusters in which the reaction products are ionized with little or no fragmentation by 26.5 eV photons from a desktop-size 46.9 nm Ne-like Ar laser. Hf and Zr oxides are found to be much less reactive than Si or Ti oxides in the presence of EUV light. The results are relevant to the design of EUV mirror capping layers that are resistant to carbon contamination.

10.IR/VUV photoionization spectroscopy for vibrational analysis, conformational analysis, and ion chemistry of molecules and clusters

Infrared plus vacuum ultraviolet (IR/VUV) photoionization spectroscopy can be employed to elucidate the structures, properties, and unimolecular reactivities of hydrogen bonded systems. The use of VUV radiation eliminates the need for the presence of UV chromophores in the molecules, and therefore the IR/VUV technique potentially has broader applicability than the conventional IR/UV double resonance technique. This advantage results from the fact that a single VUV photon has sufficient energy to ionize molecules and clusters without the need for an intermediate state, as required for UV resonance enhanced multiphoton ionization (REMPI). A variety of chemical, physical, structural, and electronic properties determined by IR/VUV and IR/UV spectroscopic techniques can be determined. The systems studied in this context include aliphatic and aromatic alcohols, acids, and amines. Both unimolecular and clustered species can be accessed by the experimental and theoretical approaches undertaken for the rest of the program.

11. Reactions between Small Neutral Iron Oxide Clusters and Carbon Monoxide

Reactions of small *neutral* iron oxide clusters (FeO_{1-3} and $Fe_2O_{4,5}$) with carbon monoxide (CO) are investigated by experiments and first-principle calculations. Detection of the neutral clusters is through ionization with vacuum UV laser (118 nm) radiation and time-of-flight mass spectrometry. The FeO_2 and FeO_3 neutral clusters are reactive toward CO, whereas $Fe2O_4$, $Fe2O_5$, and possibly FeO are not reactive. A higher reactivity for FeO_2 [$\sigma(FeO_2 + CO) > 3 \times 10^{-17}$ cm^2] than for FeO_3 [$\sigma(FeO_3 + CO) \sim 1 \times 10^{-17}$ cm^2] is observed. Density functional theory calculations are carried out to interpret the experimental observations and to generate the reaction mechanisms. The reaction pathways with negative or very small overall barriers are identified for CO oxidation by FeO_2 and FeO_3. The lower reactivity of FeO_3 with respect to FeO_2 may be related to a spin inversion process present in the reaction of FeO_3 with CO. Significant reaction barriers are calculated for the

reactions of FeO and Fe_2O_{4-5} with CO. The DFT results are in good agreement with experimental observations. Molecular level reaction mechanisms for CO oxidation by O_2, facilitated by condensed phase iron oxides as catalysts, are proposed.

12.Experimental and theoretical study of neutral Al_mC_n and Al_mCnH_x clusters

Neutral Al_mC_n and $Al_mC_nH_x$ clusters are investigated both experimentally and theoretically for the first time. Single photon ionization through 193, 118, and 46.9 nm lasers is used to detect neutral cluster distributions through time of flight mass spectrometry (TOFMS). Al_mC_n clusters are generated through laser ablation of a mixture of Al and C powders pressed into a disk. An oscillation of the vertical ionization energies (VIEs) of Al_mC_n clusters is observed in the experiments. The VIEs of Al_mC_n clusters change as a function of the numbers of Al and C atoms in the clusters. $Al_mC_nH_x$ clusters are generated through an Al ablation plasma-hydrocarbon reaction, an Al–C ablation plasma reacting with H_2 gas, or through cold Al_mC_n clusters reacting with H_2 gas in a fast flow reactor. The VIEs of $Al_mC_nH_x$ clusters are observed to vary as a function of the number of H atoms in the clusters. Density functional theory and *ab initio* calculations are carried out to explore the structures, ionization energies, and electronic structures of the Al_mC_n and $Al_mC_nH_x$ clusters. C=C bonds are favored for the lowest energy structures for Al_mC_n clusters. H atoms can be bonded to either Al or C atoms in forming $Al_mC_nH_x$ clusters, with little difference in energy. Electron density plots of the highest occupied molecular orbitals (HOMOs) for closed shell species and the singly occupied molecular orbitals (SOMOs) for open shell species of Al_mC_n and $Al_mC_nH_x$ clusters are presented and described to help understand the physical and chemical properties of the observed species. VIEs do not simply depend on open or closed shell valence electron configurations, but also depend on the electronic structure details of the clusters. The calculational results provide a good and consistent explanation for the experimental observations, and are in general agreement with them. All calculated clusters are found to have a number of low lying isomeric structures.

List of Publications

S. Heinbuch, F. Dong, J. J. Rocca, and E. R. Bernstein, "Experimental and Theoretical Studies of Reactions of Neutral Vanadium and Tantalum Oxide Clusters with NO and NH_3," J. Chem. Phys. 133,174314(2010).

Y. Xie, F. Dong, S. Heinbuch, J. J. Rocca, and E. R. Bernstein, "Oxidation Reactions on Neutral Cobalt Oxide Clusters: Experimental and Theoretical Studies," Phys. Chem. Chem. Phys. 12, 947 (2010).

J. -W. Shin and E. R. Bernstein, "Application of IR/VUV Photoionization Spectroscopy for Vibrational Analysis, Conformational Analysis, and Ion Chemistry of Molecules and Clusters," (Invited Review) Trends Appl. Spectrosc. 7, 47 (2009).

F. Dong, S. Heinbuch, Y. Xie, J. J. Rocca, and E. R. Bernstein, "Reactions of Neutral Vanadium Oxide Clusters with Methanol," J. Phys. Chem. A 113, 3029 (2009).

Y. Xie, F. Dong, S. Heinbuch, J. J. Rocca, and E. R. Bernstein, "Investigation of the Reactions of Small Neutral Iron Oxide Clusters with Methanol," J. Chem. Phys. 130, 114306 (2009).

F. Dong, S. Heinbuch, Y. Xie, J. J. Rocca, and E. R. Bernstein, "C=C Bond Cleavage on $VO_3(V_2O_5)n$ Clusters," J. Am. Chem. Soc. 131, 1057 (2009).

S. -G. He, Y. Xie, F. Dong, S. Heinbuch, E. Jakubikova, J. J. Rocca, and E. R. Bernstein, "Reactions of Sulfur Dioxide with Neutral Vanadium Oxide Clusters in the Gas Phase. II. Experimental Study Employing Single-Photon Ionization," J. Phys. Chem. A 112, 11067 (2008)

W. Xue, Z. -C. Wang, S. G. He, Y. Xie, and E. R. Bernstein, "Experimental and Theoretical Study of the Reactions between Small Neutral Iron Oxide Clusters and Carbon Monoxide." J. Am. Chem. Soc.

Z. -C. Wang, W. Xue, Y. -P. Ma, X. -L. Ding, S. -G. He, F. Dong, S. Heinbuch, J. J. Rocca, and E. R. Bernstein, " Partial Oxidation of Propylene Catalyzed by VO_3 Clusters: A DFT Study" J. Phys. Chem. A 112, 5984 (2008).

S. Heinbuch, F. Dong, J. J. Rocca, and E. R. Bernstein, "Gas Phase Study of the Reactivity of Optical Coating Materials With Hydrocarbons Using a Desk-size EUV Laser." J. Opt. Soc. Am. B 25, B85 (2008).

F. Dong, S. Heinbuch, Y. Xie, J. J. Rocca, and E. R. Bernstein, "Experimental and Theoretical Study of the Reactions Between Neutral Vanadium Oxide Clusters and Ethane, Ethylene, and Acetylene." J. Am. Chem. Soc. 130, 1932 (2008).

E. Jakubikova and E. R. Bernstein, "Reactions of Sulfur Dioxide with Neutral Vanadium Oxide Clusters in the Gas Phase. I. Density Functional Theory Study," J. Phys. Chem. A 111, 13339 (2007).

S. Heinbuch, F. Dong, J. J. Rocca, and E. R. Bernstein, "Single Photon Ionization of Hydrogen Bonded Clusters with a Soft X-ray Laser: $(HCOOH)_x$ and $(HCOOH)_y(H_2O)_z$," J. Chem. Phys. 126, 244301 (2007).

E. Jakubikova, A. K. Rappe, and E. R. Bernstein, "Density Functional Theory Study of Small Vanadium Oxide Clusters," J. Phys. Chem. A. 111, 12938 (2007).

S. G. He, Y. Xie, and E. R. Bernstein, "Formation, Detection, and Stability Studies on the Neutral Vanadium Sulfide Clusters," J. Chem. Phys. 126, 194315 (2007).

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